

## Core-softened Fluids, Water-like Anomalies and the Liquid-Liquid Critical Points

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Molecular dynamics simulations are used to examine the relationship between water-like anomalies and the liquid-liquid critical point in a family of model fluids with multi-Gaussian, core-softened pair interactions. The core-softened pair interactions have two length scales, such that the longer length scale associated with a shallow, attractive well is kept constant while the shorter length scale associated with the repulsive shoulder is varied from an inflection point to a minimum of progressively increasing depth. The maximum depth of the shoulder well is chosen so that the resulting potential reproduces the oxygen-oxygen radial distribution function of the ST4 model of water. As the shoulder well depth increases, the pressure required to form the high density liquid decreases and the temperature up to which the high-density liquid is stable increases, resulting in the shift of the liquid-liquid critical point to much lower pressures and higher temperatures. To understand the entropic effects associated with the changes in the interaction potential, the pair correlation entropy is computed to show that the excess entropy anomaly diminishes when the shoulder well depth increases. Excess entropy scaling of diffusivity in this class of fluids is demonstrated, showing that decreasing strength of the excess entropy anomaly with increasing shoulder depth results in the progressive loss of water-like thermodynamic, structural and transport anomalies. Instantaneous normal mode analysis was used to index the overall curvature distribution of the fluid and the fraction of imaginary frequency modes was shown to correlate well with the anomalous behavior of the diffusivity and the pair correlation entropy. The results suggest in the case of core-softened potentials, in addition to the presence of two length scales, energetic and entropic effects associated with local minima and curvatures of the pair interaction play an important role in determining the presence of water-like anomalies and the liquid-liquid phase transition.